Can Pb-free Halide Double Perovskites Support High-efficiency Solar Cells?

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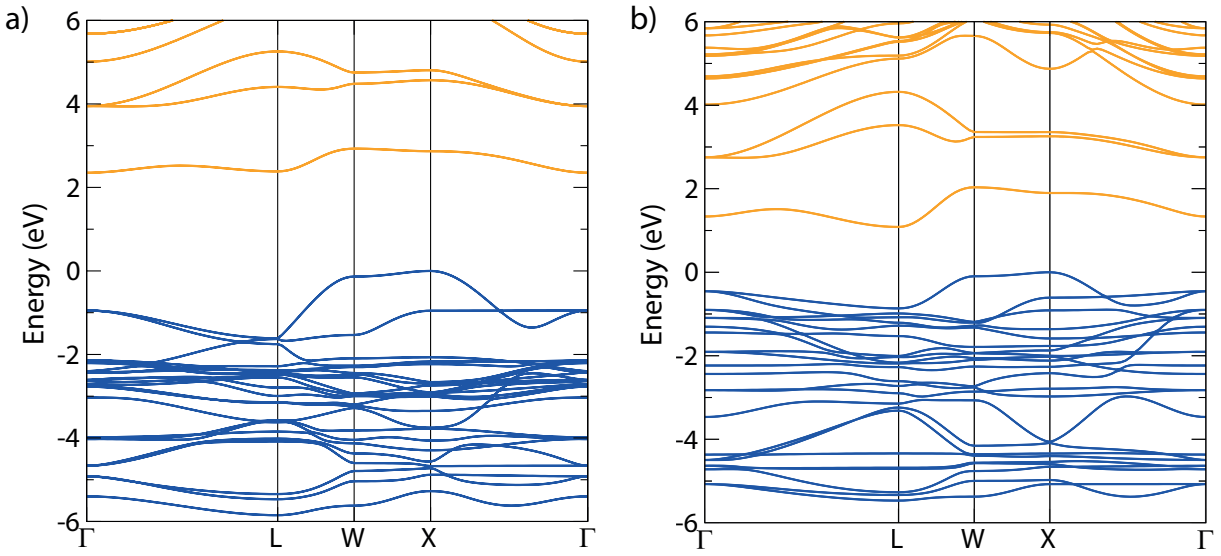

Figure 1: HSE06+SOC band structures of a) $Cs_2AgBiCl_6$ and b) Cs_2AgBiI_6, with valence band in blue, and conduction band in orange. Valence band maximum (VBM) is set to 0 eV.

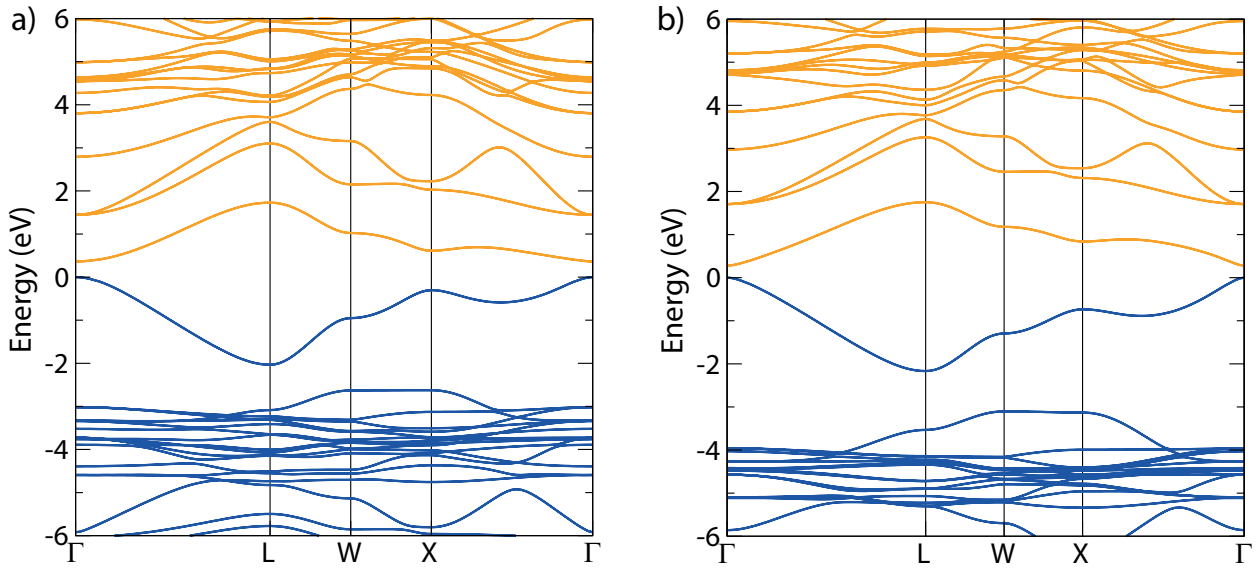

Figure 2: HSE06+SOC band structures of a) $Cs_2InBiCl_6$ and b) $Cs_2InBiBr_6$, with valence band in blue, and conduction band in orange. VBM is set to 0 eV.

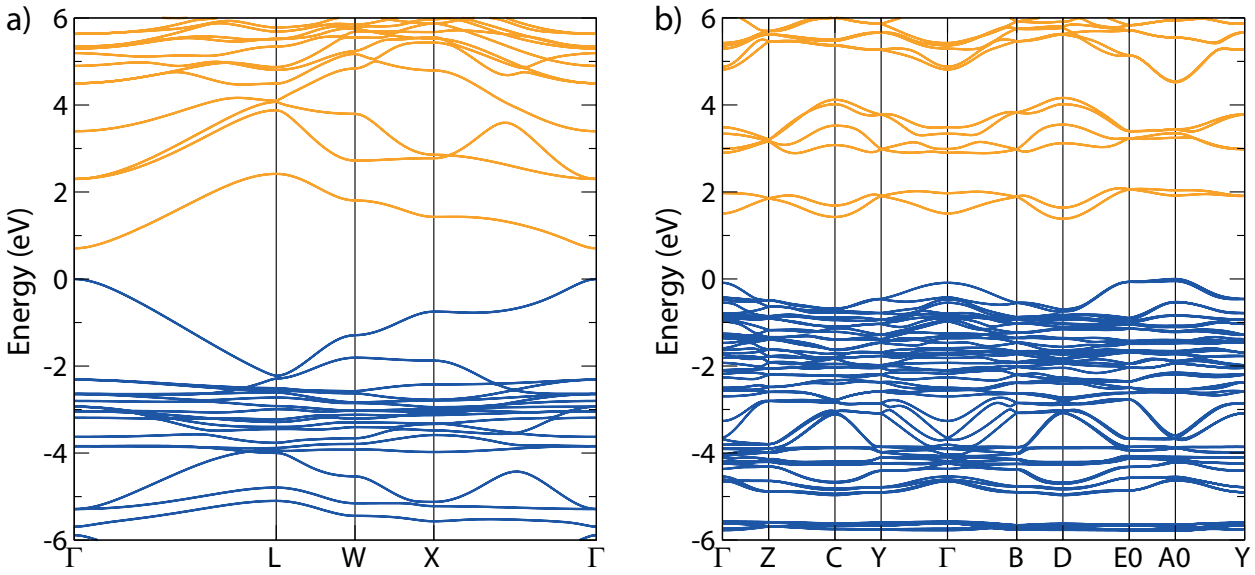

Figure 3: HSE06+SOC band structures of a) $Cs_2TlBiBr_6$ and b) $(CH_3NH_3)_2AgBiI_6$ (starting from the orthorhombic $(CH_3NH_3)PbI_3$ structure)[1] with valence band in blue, and conduction band in orange. The high-symmetry path used for $(CH_3NH_3)_2AgBiI_6$ uses k-points from the lowered C-centered monoclinic space group. VBM is set to 0 eV.

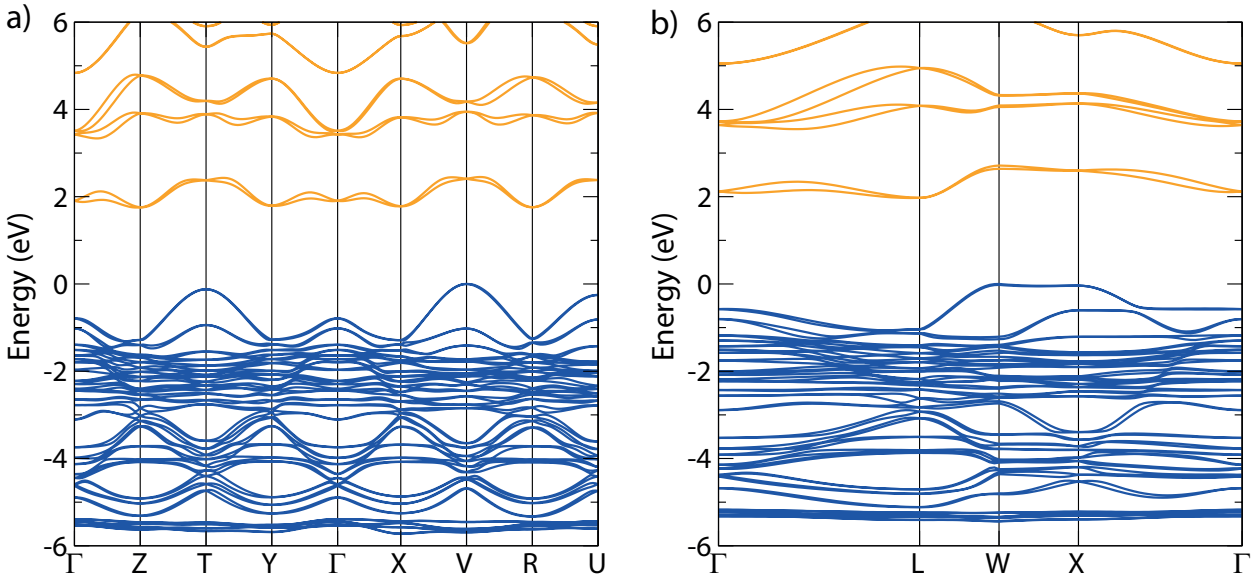

Figure 4: HSE06+SOC band structures of $(CH_3NH_3)_2AgBiBr_6$ (starting from the primitive cell of the cubic $Cs_2AgBiBr_6$ structure),[2] with valence band in blue, and conduction band in orange. a) uses the high-symmetry path of the lowered primitive triclinic space group, while b) uses the F-centered cubic high-symmetry lines. VBM is set to 0 eV.

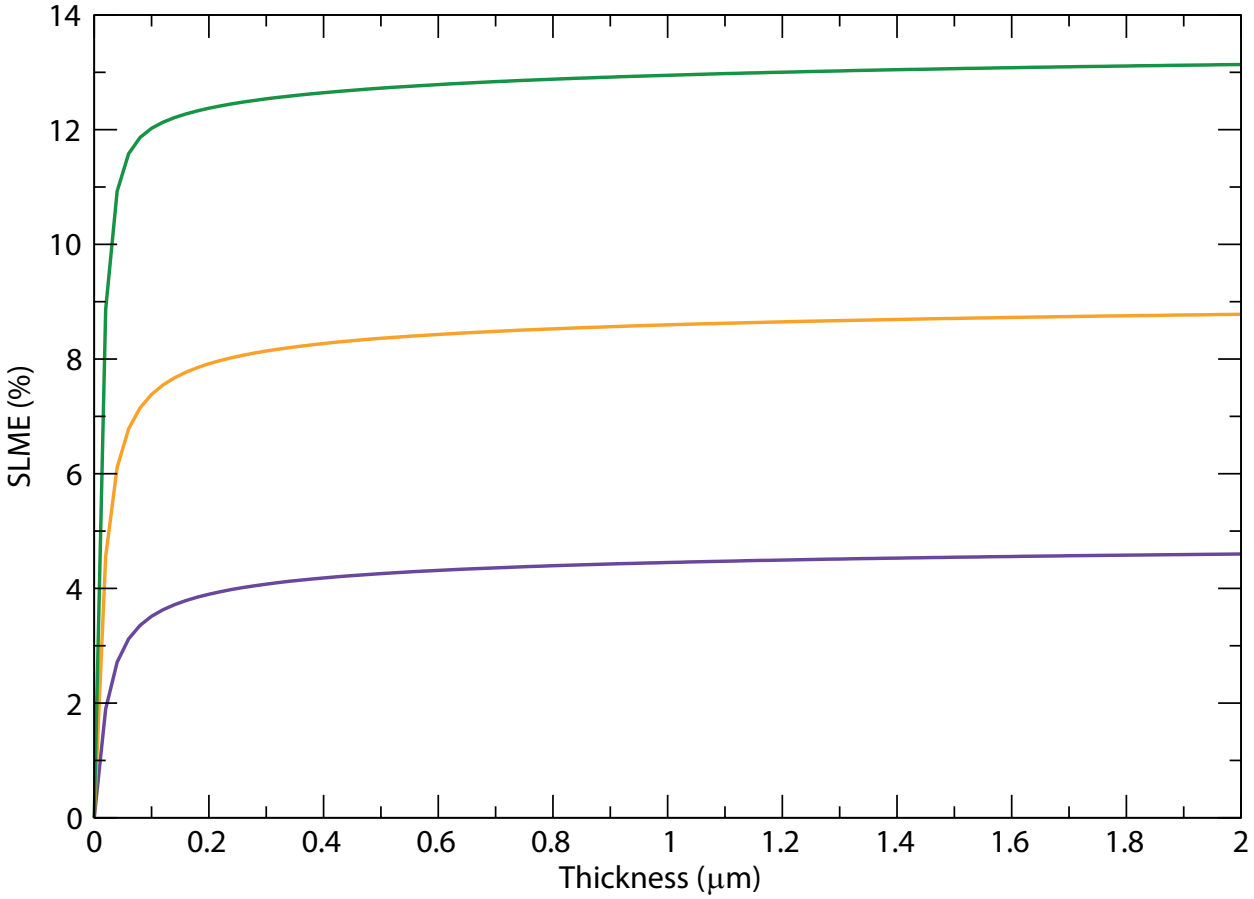

Figure 5: Plot of the predicted SLMEs against film thickness for $Cs_2AgBiCl_6$ (green), $Cs_2AgBiBr_6$ (orange) and Cs_2AgBiI_6 (purple).

References

(1) Weller, M. T.; Weber, O. J.; Henry, P. F.; Pumpo, M. D.; Hansen, T. C. Complete structure and cation orientation in the perovskite photovoltaic methylammonium lead iodide between 100 and 352 K. *Chemical Communications* **2015**, *51*, 4180–4183.

(2) McClure, E. T.; Ball, M. R.; Windl, W.; Woodward, P. M. Cs2AgBiX6 (X = Br, Cl): New Visible Light Absorbing, Lead-Free Halide Perovskite Semiconductors. *Chemistry of Materials* **2016**, *28*, 1348–1354.